Time Step Determination for PDEs with Applications to Programs Written with Overture
Draft version.

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Abstract: We describe the practical aspects of computing the time step for a PDE that has been discretized on a curvilinear grid. Sample programs are given using Overture.

1   ODEs

Consider the stability of the model problem (ODE initial value problem)

$$y' = ay , \quad a \in \mathbf{C}$$
$$y(0) = y_0$$

Suppose we discretize with some method

$$v^{n+1} = \mathcal{S}(a\Delta t, v^n, v^{n-1}, ...) \tag{1}$$
$$\lambda \equiv a\Delta t \tag{2}$$

The region of absolute stability for the scheme (1) is defined to be the region in the complex plane for $\lambda = a\Delta t$ such that the solution v^n remains bounded for all initial data v^0,

$$\mathcal{A} = \{\lambda \in \mathbf{C} : |v^n| \le K \quad \forall n, \quad \forall v^0\}$$

Example: The forward Euler scheme

$$v^{n+1} = v^n + a\Delta t v^n \tag{3}$$
$$\implies v^{n+1} = (1 + \lambda)^{n+1} v^0 \tag{4}$$

is stable provided

$$|1 + \lambda| \le 1$$

This defines the region interior to the circle in the complex plane centered at -1 with radius 1.

Example: The backward Euler scheme

$$v^{n+1} = v^n + a\Delta t v^{n+1} \tag{5}$$

$$\implies v^{n+1} = \frac{1}{(1-\lambda)^{n+1}}v^0 \tag{6}$$

is stable provided

$$\frac{1}{|1-\lambda|} \leq 1$$

This defines the region exterior to the circle in the complex plane centered at $+1$ with radius 1.

Example: The trapezoidal scheme

$$v^{n+1} = v^n + \frac{a\Delta t}{2}\left(v^n + v^{n+1}\right) \tag{7}$$

$$\implies v^{n+1} = \left(\frac{1+\frac{1}{2}\lambda}{1-\frac{1}{2}\lambda}\right)^{n+1} v^0 \tag{8}$$

is stable provided

$$\left|\frac{1+\frac{1}{2}\lambda}{1-\frac{1}{2}\lambda}\right| \leq 1$$

This defines the region $\Re(\lambda) \leq 0$, the left half plane.

Example: The midpoint rule (modified Euler) scheme

$$v^{n+\frac{1}{2}} = v^n + \frac{a\Delta t}{2}v^n \tag{9}$$

$$v^{n+1} = v^n + a\Delta t[v^{n+\frac{1}{2}}] \tag{10}$$

$$\implies v^{n+1} = [1 + \lambda + \frac{1}{2}\lambda^2]^{n+1}v^0 \tag{11}$$

is stable provided

$$\left|1 + \lambda + \frac{1}{2}\lambda^2\right| \leq 1$$

This defines an elliptical like region that extends to -2 on the real axis and passes through the point $(-1, \sqrt{3})$. See figure ??.

Example: The Leap-frog scheme

$$v^{n+2} = v^n + 2a\Delta t[v^{n+1}] \tag{12}$$

is a two level scheme that we solve by trying $v^n = \kappa^n$ which implies

$$\kappa = ...$$

is stable provided κ lies on the imaginary axis and ...

2 Fourier or von Neumann Stability Analysis for PDEs

Recall the discrete fourier transform and its inverse

$$v_j = \sum_{\omega=N/2}^{N/2-1} \hat{v}_\omega e^{2\pi i \omega x_j}$$

$$\hat{v}_\omega = \sum_{j=0}^{N-1} v_j e^{-2\pi i \omega x_j} h$$

2.1 Diffusion Equation

Now consider the parabolic PDE ($\nu > 0$)

$$u_t = \nu u_{xx} \qquad x \in (0,1)$$
$$u(x,0) = u_0(x)$$
$$u \text{ and } u_0 \text{are } 1\text{-periodic}$$

Introduce a grid on the interval $[0,1]$, and discretize in space

$$\frac{d}{dt}v_j(t) = \nu D_+ D_- v_j \qquad j = 0,1,...,N-1$$
$$v_j(0) = u_0(x_j)$$
$$x_j = jh \qquad h = 1/N$$
$$v(x_j) = v(x_{j+N})$$

To analyse the stability of this scheme we fourier transform,

$$\frac{d}{dt}\hat{v}_\omega(t) = \frac{\nu}{h^2}(e^{2\pi i \omega h} - 2 + e^{-2\pi i \omega h})\hat{v}_\omega$$
$$= -4\frac{\nu}{h^2}\sin^2(\xi/2)\hat{v}_\omega$$

where

$$\xi = 2\pi\omega h \qquad \omega = -N/2,...,N/2-1$$
$$-\pi \le \xi < \pi$$

Define

$$\hat{Q}(\xi) = -4\frac{\nu\Delta t}{h^2}\sin^2(\xi/2)$$

The scheme has been reduced to an ODE with $\lambda = \hat{Q}(\xi)$. Any particular time-stepping routine will be stable provided $\hat{Q}(\xi)$ lies in the stability region for all $-\pi \le \xi < \pi$.
Example: For forward Euler time-stepping the scheme is stable provided

$$|1 + \hat{Q}(\xi)| \le 1, \qquad -\pi \le \xi < \pi$$

which implies

$$\frac{\nu\Delta t}{h^2} \le \frac{1}{2}$$

Example: If we discretize with backward-Euler, then we require

$$\frac{1}{1 + 4\frac{\nu\Delta t}{h^2}\sin^2(\xi/2)} \le 1, \qquad -\pi \le \xi < \pi$$

and thus the scheme stable for any value of $\Delta t \ge 0$, (since $\nu > 0$).

2.2 Convection Diffusion Equation

Consider the convection diffusion equation

$$u_t + au_x = \nu_{xx}$$

Discretize in space,

$$\frac{d}{dt}v_j = -aD_0 v_j(t) + \nu D_+ D_- v_j(t)$$

and Fourier transform gives

$$\frac{d}{dt}\hat{v}_\omega = [-\frac{a}{2h}(e^{i\xi} - e^{-i\xi}) + \frac{\nu}{h^2}(e^{i\xi} - 2 + e^{-i\xi})]\hat{v}_\omega$$

Define

$$\hat{Q} = \left\{-\frac{ia}{h}\sin(\xi) - \frac{4\nu}{h^2}\sin^2(\xi/2)\right\}\Delta t$$

A particular time stepping scheme will be stable provided $\hat{Q}$ lies in its stability region.

To simplify the discussion suppose that the stability region is contained in an ellipse:

$$\text{Stability Region:} \quad \mathcal{A}: \quad \left(\frac{x}{\alpha_0}\right)^2 + \left(\frac{y}{\beta_0}\right)^2 \leq 1$$

If the real and imaginary parts of $\hat{Q}$ are

$$\hat{Q} = \Re(\hat{Q}) + i\,\Im(\hat{Q})$$

then the scheme is stable provided

$$\left(\frac{\Re(\hat{Q})}{\alpha_0}\right)^2 + \left(\frac{\Im(\hat{Q})}{\beta_0}\right)^2 \leq 1$$

$$\implies \left(\frac{4\nu\Delta t}{\alpha_0 h^2}\sin^2(\xi/2)\right)^2 + \left(\frac{a\Delta t}{h\beta_0}\sin(\xi)\right)^2 \leq 1$$

A sufficient condition is

$$\left(\frac{4\nu\Delta t}{\alpha_0 h^2}\right)^2 + \left(\frac{a\Delta t}{h\beta_0}\right)^2 \leq 1$$

which implies

$$\Delta t \leq \left[\left(\frac{4\nu}{\alpha_0 h^2}\right)^2 + \left(\frac{a}{h\beta_0}\right)^2\right]^{-\frac{1}{2}}$$

3 Variable Coefficients

Now consider the convection diffusion equation with variable coefficients

$$u_t + a(x)u_x = \nu(x)u_{xx}$$

If we discretize in space we get

$$\frac{d}{dt}v = -a(x_j)D_0 v_j(t) + \nu(x_j)D_+D_-v_j(t)$$

To simplify the analysis we freeze the coefficients

$$\frac{d}{dt}v = -a_0 D_0 v_j(t) + \nu_0 D_+D_-v_j(t)$$

and Fourier transform as before giving

$$\hat{Q}(\xi) = \left\{-\frac{ia_0}{h}\sin(\xi) - \frac{4\nu_0}{h^2}\sin^2(\xi/2)\right\}\Delta t$$

Now we unfreeze the coefficients

$$\hat{Q}(\xi,x) = \left\{-\frac{ia(x)}{h}\sin(\xi) - \frac{4\nu(x)}{h^2}\sin^2(\xi/2)\right\}\Delta t$$

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and impose the condition that $\hat{Q}(\xi, x)$ lies in the stability region of the time-stepping method for $-\pi \leq \xi < \pi$ and $0 \leq x \leq 1$.

A "sufficient" condition is thus

$$\Delta t \leq \min_{0 \leq x \leq 1} \left[\left(\frac{4\nu(x)}{\alpha_0 h^2} \right)^2 + \left(\frac{a(x)}{h\beta_0} \right)^2 \right]^{-\frac{1}{2}}$$

Result: This approach, although not strictly rigorous, usually works in practice. Why? Instabilities are usually high-frequencies so as long as the coefficients vary smoothly it is a reasonable approximation to locally freeze them.

4   Stability in Multiple Space Dimensions

Consider the 2D heat equation

$$u_t = \nu(u_{xx} + u_{yy}) \qquad 0 \leq x, y \leq 1$$
$$u(x, y, 0) = u_0(x, y)$$
$$u \text{ and } u_0 \text{ 1-periodic}$$

Discretize in space

$$\frac{d}{dt} v_{\mu\nu} = \nu(D_{+x}D_{-x}v_{\mu\nu} + D_{+y}D_{-y}v_{\mu\nu}) \qquad \mu = 0, 1, ..., N-1 \quad \nu = 0, 1, ..., N-1$$

Now Fourier transform

$$v_{\mu\nu} = \sum_{\mu,\nu} \hat{v}_\omega e^{i\mu\xi_x} e^{i\nu\xi_y}$$

$$\xi_x = 2\pi\omega_x x_\mu \qquad \xi_y = 2\pi\omega_y y_\nu , \qquad \omega = (\omega_x, \omega_y)$$
$$-\pi \leq \xi_x, \xi_y < \pi$$

giving

$$\frac{d}{dt}\hat{v}_\omega = \nu \left(-\frac{4\sin^2(\xi_x/2)}{h_x^2} - \frac{4\sin^2(\xi_y/2)}{h_y^2} \right) \hat{v}_\omega$$

and the scheme will be stable provided

$$\hat{Q}(\xi_x, \xi_y) = -4\nu\Delta t \left(\frac{\sin^2(\xi_x/2)}{h_x^2} + \frac{\sin^2(\xi_y/2)}{h_y^2} \right)$$

is in the stability region.

Example: For Forward Euler time stepping we require $|1 + \hat{Q}| \leq 1$, or since $\hat{Q} \in \mathbf{R}$ we need $-2 \leq \hat{Q} \leq 0$ and thus

$$\Delta t \leq \frac{1}{2\nu} \left[\frac{1}{h_x^2} + \frac{1}{h_y^2} \right]^{-1}$$

5   Variable Coefficients and a Curvilinear Grid

Now consider the problem of determining the time step for an equation discretized on a curvilinear grid using the *mapping method*.

Given the equation

$$u_t + a(\mathbf{x})u_x + b(\mathbf{x})u_y = \nu(\mathbf{x})(u_{xx} + u_{yy}) \qquad \mathbf{x} = (x, y) \qquad 0 \leq x, y \leq 1$$

Suppose we want to discretize on a region defined by the mapping $\mathbf{x} = \mathbf{g}(\mathbf{r})$ where $\mathbf{r}$ are the unit square coordinates, $\mathbf{r} = (r_1, r_2) = (r, s)$. To discretize we first transform to the unit square coordinates,

$$u(\mathbf{x}) = u(\mathbf{g}(\mathbf{r})) \equiv U(\mathbf{r})$$

and compute derivatives using the chain rule

$$\frac{\partial u}{\partial x_i} = \sum_{\mu} \frac{\partial r_\mu}{\partial x_i} \frac{\partial U}{\partial r_\mu}$$

Example: In 2D,

$$u_x = \frac{\partial r_1}{\partial x} \frac{\partial U}{\partial r_1} + \frac{\partial r_2}{\partial x} \frac{\partial U}{\partial r_2}$$

$$u_{xx} = \left(\frac{\partial r_1}{\partial x}\right)^2 \frac{\partial^2 U}{\partial r_1^2} + \left(\frac{\partial r_2}{\partial x}\right)^2 \frac{\partial^2 U}{\partial r_2^2} + 2\frac{\partial r_1}{\partial x} \frac{\partial r_2}{\partial x} \frac{\partial^2 U}{\partial r_1 \partial r_2} + \frac{\partial^2 r_1}{\partial x^2} \frac{\partial U}{\partial r_1} + \frac{\partial^2 r_2}{\partial x^2} \frac{\partial U}{\partial r_2}$$

Thus our equation transforms to

$$U_t + \tilde{a}(\mathbf{r})U_{r_1} + \tilde{b}(\mathbf{r})U_{r_2} = \tilde{\nu}_{11}(\mathbf{r})U_{r_1 r_1} + \tilde{\nu}_{12}(\mathbf{r})U_{r_1 r_2} + \tilde{\nu}_{22}(\mathbf{r})U_{r_2 r_2}$$

where

$$\tilde{a}(\mathbf{r}) = \frac{\partial r_1}{\partial x}a(\mathbf{x}) + \frac{\partial r_1}{\partial y}b(\mathbf{x}) - \left(\frac{\partial^2 r_1}{\partial x^2} + \frac{\partial^2 r_1}{\partial y^2}\right)\nu(\mathbf{x})$$

$$\tilde{b}(\mathbf{r}) = \frac{\partial r_2}{\partial x}a(\mathbf{x}) + \frac{\partial r_2}{\partial y}b(\mathbf{x}) - \left(\frac{\partial^2 r_2}{\partial x^2} + \frac{\partial^2 r_2}{\partial y^2}\right)\nu(\mathbf{x})$$

$$\nu_{11}(\mathbf{r}) = \nu(x)\left[\left(\frac{\partial r_1}{\partial x}\right)^2 + \left(\frac{\partial r_1}{\partial y}\right)^2\right]$$

$$\nu_{12}(\mathbf{r}) = \nu(x)\left[2\frac{\partial r_1}{\partial x}\frac{\partial r_2}{\partial x} + 2\frac{\partial r_1}{\partial y}\frac{\partial r_2}{\partial y}\right]$$

$$\nu_{22}(\mathbf{r}) = \nu(x)\left[\left(\frac{\partial r_2}{\partial x}\right)^2 + \left(\frac{\partial r_2}{\partial y}\right)^2\right]$$

Now discretize in space

$$\frac{d}{dt}v_{\mu\nu} + \tilde{a}D_{0r}v_{\mu\nu} + \tilde{b}D_{0s}v_{\mu\nu} = \nu_{11}D_{+r}D_{-r}v_{\mu\nu} + \nu_{12}D_{0r}D_{0s}v_{\mu\nu}) + \nu_{22}D_{+s}D_{-s}v_{\mu\nu})$$

If we freeze coefficients and Fourier transform we get

$$\frac{d}{dt}\hat{v}_\omega = \left\{-\frac{i\tilde{a}}{h_1}\sin(\xi_1) - \frac{i\tilde{b}}{h_2}\sin(\xi_2) - \frac{4\nu_{11}\sin^2(\xi_1/2)}{h_1^2} - \frac{\nu_{12}\sin(\xi_1)\sin(\xi_2)}{h_1 h_2} - \frac{4\nu_{22}\sin^2(\xi_2/2)}{h_2^2}\right\}\hat{v}_\omega$$

$$= \hat{Q}(\xi_1, \xi_2)$$

Now unfreeze the coefficients and if we assume, as before, that the stability region is an ellipse, then a stability condition is

$$\Delta t \leq \min_{0 \leq r_1, r_2 \leq 1}\left\{\left[\frac{1}{\beta_0}\left(\frac{|\tilde{a}|}{h_1} + \frac{|\tilde{b}|}{h_2}\right)\right]^2 + \left[\frac{1}{\alpha_0}\left(\frac{4\nu_{11}}{h_1^2} + \frac{|\nu_{12}|}{h_1 h_2} + \frac{4\nu_{22}}{h_2^2}\right)\right]^2\right\}^{-\frac{1}{2}}$$

5.1 Overture code for determining the time-step for a 2D scalar convection diffusion equation

Here is a function that computes the time step for a convection diffussion equation, `Overture/primer/getDt.C`, it is used by `Overture/primer/mappedGridExample6.C`

6 Systems of Equations

Consider now the system of equations

$$\frac{\partial \mathbf{u}}{\partial t} + A\frac{\partial \mathbf{u}}{\partial x} = \nu\frac{\partial^2 \mathbf{u}}{\partial x^2}$$

Suppose that the matrix A is diagonalizable

$$A = S^{-1}\Lambda S \ , \ \Lambda = \begin{bmatrix} \lambda_1 & 0 & \cdots \\ 0 & \lambda_2 & \cdots \\ \cdots & 0 & \lambda_n \end{bmatrix}$$

Now if we discretize in space

$$\frac{d\mathbf{v}_j}{dt} = -AD_0\mathbf{v}_j + \nu D_+ D_- \mathbf{v}_j$$

and Fourier transform

$$\frac{d\hat{\mathbf{v}}}{dt} = \left[-\frac{i\sin(\xi)}{h}A - \frac{4\nu \sin^2(\xi/2)}{h^2} \right]\hat{\mathbf{v}}$$

and transform to diagonal form ($\mathbf{w} = S\mathbf{v}$)

$$\frac{d\hat{\mathbf{w}}}{dt} = \left[-\frac{i\sin(\xi)}{h}\Lambda - \frac{4\nu \sin^2(\xi/2)}{h^2} \right]\hat{\mathbf{w}}$$

then defining

$$\hat{Q}(\xi, \lambda_\mu) = \left[-\frac{i\sin(\xi)}{h}\lambda_\mu - \frac{4\nu \sin^2(\xi/2)}{h^2} \right]\Delta t$$

The scheme will be stable provided $\hat{Q}(\xi, \lambda_\mu)$ lies in the stability region for all eigenvalues.

6.1 The 1D Shallow Water Equations

The Shallow water equations in one space dimension are

$$h_t + uh_x + hu_x = 0$$
$$u_t + uu_x + gh_x = 0$$

If we discretize on a uniform grid,

$$\frac{d\mathbf{v}_j}{dt} + \begin{bmatrix} u_j & h_j \\ g & u_j \end{bmatrix} D_0 \mathbf{v}_j = 0$$

$$\mathbf{v}_j = \begin{bmatrix} h_j \\ u_j \end{bmatrix}$$

Freezing coefficients and Fourier transforming

$$\frac{d\hat{\mathbf{v}}}{dt} + \begin{bmatrix} u_0 & h_0 \\ g & u_0 \end{bmatrix} \frac{i\sin(\xi)}{h}\hat{\mathbf{v}} = 0$$

The eigenvalues of

$$A = \begin{bmatrix} u_j & h_j \\ g & u_j \end{bmatrix}$$

are

$$\lambda_\pm = u_j \pm \sqrt{gh_j}$$

Define

$$\hat{Q}_\pm = \lambda_\pm \frac{i\Delta t \sin(\xi)}{h}$$

Suppose that the stability region of the time stepping scheme extends to $i\beta_0$, then we require

$$|\hat{Q}_\pm| \leq \beta_0$$

which implies

$$\Delta t \leq \beta_0 h \min_{x_i}\left\{ |u_j| + \sqrt{gh_j} \right\}^{-1}$$

7   2D systems

Consider the 2D system

$$\frac{\partial \mathbf{u}}{\partial t} + A(\mathbf{x})\frac{\partial \mathbf{u}}{\partial x} + B(\mathbf{x})\frac{\partial \mathbf{u}}{\partial y} = \nu \left(\frac{\partial^2 \mathbf{u}}{\partial x^2} + \frac{\partial^2 \mathbf{u}}{\partial y^2} \right)$$

Discretize

$$\frac{d\mathbf{v}_j}{dt} = -A(\mathbf{x}_j)D_{0x}\mathbf{v}_j - B(\mathbf{x}_j)D_{0y}\mathbf{v}_j + \nu \left(D_{-x} + D_{-x}\mathbf{v}_j + D_{-y} + D_{-y}\mathbf{v}_j \right)$$

freeze coefficeints and fourier transform

$$\frac{d\hat{v}_\omega}{dt} = \left[-\frac{i\sin(\xi_x)}{h_x}A_0 - \frac{i\sin(\xi_y)}{h_y}B_0 - 4\nu \left(\frac{\sin^2(\xi_x/2)}{h_x^2} + \frac{\sin^2(\xi_y/2)}{h_y^2} \right) \right] \hat{v}_\omega$$

Define the matrix

$$\hat{Q}(\xi_x, \xi_y; \mathbf{x}_j) = \left[-\frac{i\sin(\xi_x)}{h_x}A_(\mathbf{x}_j) - \frac{i\sin(\xi_y)}{h_y}B_(\mathbf{x}_j) - 4\nu \left(\frac{\sin^2(\xi_x/2)}{h_x^2} + \frac{\sin^2(\xi_y/2)}{h_y^2} \right) \right] \Delta t$$

It is necessary that the all the eigenvalues of $\hat{Q}(\xi_x, \xi_y; \mathbf{x}_j)$ lie within the stability region of the time stepping method.

7.1   The 2D Shallow Water Equations

The Shallow water equations in one space dimension are

$$h_t + uh_x + vh_y + h(u_x + v_y) = 0$$
$$u_t + uu_x + vu_y + gh_x = 0$$
$$v_t + uv_x + vv_y + gh_y = 0$$

If we discretize on a uniform grid,

$$\frac{d\mathbf{v}_j}{dt} + \begin{bmatrix} u_j & h_j & 0 \\ g & u_j & 0 \\ 0 & 0 & u_j \end{bmatrix} D_{0x}\mathbf{v}_j + \begin{bmatrix} v_j & 0 & h_j \\ 0 & v_j & 0 \\ g & 0 & v_j \end{bmatrix} D_{0y}\mathbf{v}_j = 0$$

$$\mathbf{v}_j = \begin{bmatrix} h_j \\ u_j \\ v_j \end{bmatrix}$$

Freezing coefficients and Fourier transforming gives

$$\frac{d\hat{v}_\omega}{dt} + \begin{bmatrix} U_0\frac{i\sin(\xi_x)}{h_x} + V_0\frac{i\sin(\xi_y)}{h_y} & H_0\frac{i\sin(\xi_x)}{h_x} & H_0\frac{i\sin(\xi_y)}{h_y} \\ g\frac{i\sin(\xi_x)}{h_x} & U_0\frac{i\sin(\xi_x)}{h_x} + V_0\frac{i\sin(\xi_y)}{h_y} & 0 \\ g\frac{i\sin(\xi_y)}{h_y} & 0 & U_0\frac{i\sin(\xi_x)}{h_x} + V_0\frac{i\sin(\xi_y)}{h_y} \end{bmatrix} \hat{v}_\omega$$

The eigenvalues are

$$\lambda_1 = i \left(U_0\frac{\sin(\xi_x)}{h_x} + V_0\frac{\sin(\xi_y)}{h_y} \right)$$

$$\lambda_{2,3} = i \left[U_0\frac{\sin(\xi_x)}{h_x} + V_0\frac{\sin(\xi_y)}{h_y} \pm \sqrt{gH_0} \left\{ \left(\frac{\sin(\xi_x)}{h_x} \right)^2 + \left(\frac{\sin(\xi_y)}{h_y} \right) \right\}^{\frac{1}{2}} \right]$$